300 °K to the value of $b = 5$ (computed value) at 4.2 °K. This is indeed consistent with the observed V_{PME}-vs-B data for T at 300 and 4.2 °K. The change in mobility ratio with temperature has also been observed in InSb.[5]

Figure 2 illustrates the plot of (V_{PME}/B) vs $\Delta G/G_0$ for $T = 300$, 77, 21, and 4.2 °K. The results (slope of this plot is one) at all temperatures show that no trapping effect is involved in the entire temperature range.[6,7] It is noted in Fig. 4 that the deviation from linearity [as is predicted by Eq. (5)] at higher magnetic field is due to the fact that the photoconductance becomes magnetic field dependent as B is increased.

IV. CONCLUSIONS

Experimental study of the PME and PC effects in n-type InAs single crystals has been extended from room temperature down to 4.2 °K. The results are in good agreement with the theory developed previously. Carrier lifetimes and mobilities are deduced from the present results. Measurements of the PME and Hall effect at low temperatures enable us to determine both the majority and minority carrier mobilities in n-type InAs. Study of the PME and PC effects show that no trapping is involved in the entire temperature range for the present samples.

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Phonon Dispersion in Noble Metals

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The phonon dispersion relations in the three symmetry directions of the noble metals copper, silver, and gold at room temperature have been determined from a model for the lattice dynamics of metals recently propounded by Chéveau. The results agree reasonably well with recent neutron scattering experiments.

The lattice dynamics of metallic crystals has been the subject of investigation by many theoretical and experimental workers over the past several years.[1] In the last few years, a number of models[2–5] have been developed for studying phonon dispersion in cubic metals, considering explicitly the presence of conduction electrons. Many of them, however, have not been able to stand the test of recent neutron scattering experiments. For example, the recent model of Krebs[5] satisfies the symmetry requirements, but suffers from a serious lack of internal equilibrium and necessitates external forces to maintain the system in equilibrium. Quite recently Chéveau[6] has propounded a model for the lattice dynamics of cubic metals which is free from these discrepancies. It satisfies the symmetry properties of a cubic lattice by using Lax's[7] expression for the electron-ion interaction contribution and preserves internal equilibrium without recourse to external forces. The ion-ion interaction is described by the first two terms in the Taylor expansion of the potential energy. This model has furnished a reasonably satisfactory description of the lattice vibrations in alkali metals,[8] and of the temperature variations of the thermal expansion, Debye-Waller factors, and transport properties of a number of cubic metals.[9,10] In this paper we report a study of phonon dispersion relations in noble metals on the Chéveau model. The motivation for this study was the recent appearance of detailed phonon dispersion curves for copper[11–13] and silver[14,15] from experiments on coherent inelastic neutron scattering.

The secular equation determining the angular frequencies ω of the normal modes of vibration in a cubic metal can be written as

$$|M(\vec{q}) - m\,\omega^2 I| = 0\,, \tag{1}$$

where m is the mass of an atom in the lattice and

TABLE I. Constants for the noble metals used in the calculation.

Metal	Elastic constants (10^{11} dyn/cm^2) C_{11}	C_{12}	C_{44}	Density (g/cm^3)	Lattice parameter (Å)
Copper[a]	16.839	12.142	7.539	8.96	3.616
Silver[b]	12.399	9.367	4.612	10.49	4.080
Gold[b]	19.234	16.314	4.195	19.32	4.070

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I is the unit matrix of order 3. Using the model of Chéveau, the elements of the dynamical matrix $M(\vec{q})$ for a face-centered cubic lattice can be written as

$$M_{ii}(\vec{q}) = 4(\alpha_1+\alpha_2)(2 - C_i C_j - C_i C_k) + 4\alpha_1(1 - C_j C_k) + 2a^3 \lambda^2(0) K_e \sum_{\vec{K}} \left(\frac{(\vec{q}+\vec{K})_i (\vec{q}+\vec{K})_i}{|\vec{q}+\vec{K}|^2 + \lambda^2(|\vec{q}+\vec{K}|/2k_F)} - \frac{K_i K_i}{|\vec{K}|^2 + \lambda^2(|\vec{K}|/2k_F)} \right) , \tag{2a}$$

$$M_{ij}(\vec{q}) = 4\alpha_2 S_i S_j + 2a^3 \lambda^2(0) K_e \sum_{\vec{K}} \left(\frac{(\vec{q}+\vec{K})_i (\vec{q}+\vec{K})_j}{|\vec{q}+\vec{K}|^2 + \lambda^2(|\vec{q}+\vec{K}|/2k_F)} - \frac{K_i K_j}{|\vec{K}|^2 + \lambda^2(|\vec{K}|/2k_F)} \right) , \tag{2b}$$

where $S_i = \sin(q_i a)$ and $C_i = \cos(q_i a)$. Here q_i is the ith Cartesian component of the phonon wave vector $\vec{q}$, $\vec{K}$ is the reciprocal-lattice vector, kF is the Fermi wave number, a is the semilattice parameter, and $\lambda(k)$ is the Thomas-Fermi screening parameter as modified by Langer and Vosko.[16] The parameters α_1 and α_2 are the first two derivatives of the potential energy at the nearest-neighbor separation, and the factor K_e arises from the electron-ion interaction. Considering the long-wavelength limit of (1), the parameters α_1, α_2, and K_e can be related to the three independent elastic constants of a cubic metal through the relations

$$\alpha_1 = \tfrac{1}{2}a(C_{11} - C_{12} - C_{44}) ,$$
$$\alpha_2 = -a(C_{11} - C_{12} - 2C_{44}) , \tag{3}$$
$$K_e = 2C_{11} - C_{12} - 3C_{44} .$$

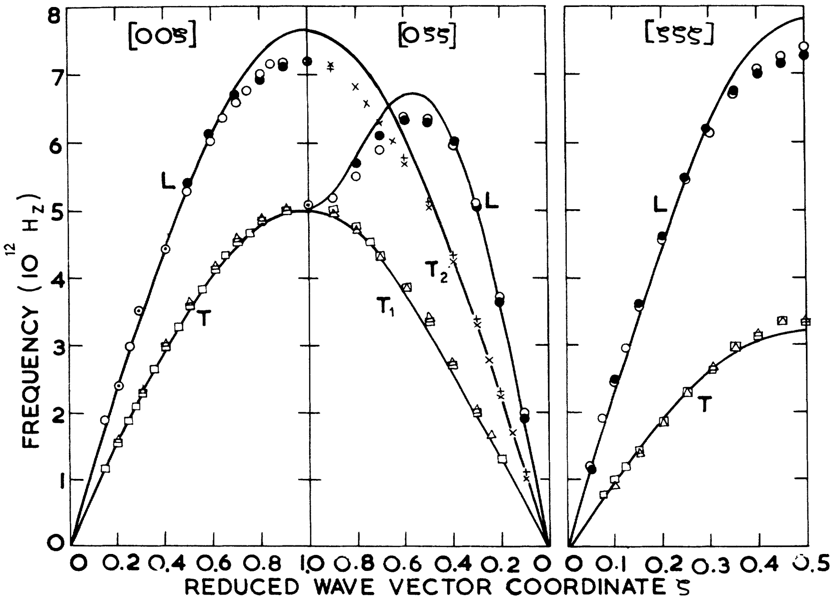

FIG. 1. Phonon dispersion curves for copper at room temperature in the three symmetry directions. Experimental points: ○, □, × (Svensson *et al.*); ●, △, + (Nicklow *et al.*).

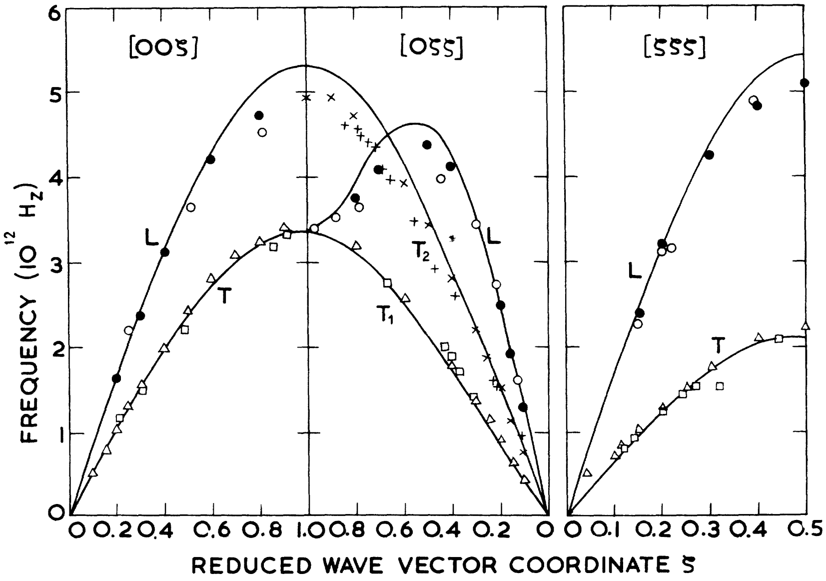

FIG. 2. Phonon dispersion curves for silver at room temperature in the three symmetry directions. Experimental points: ○, □, + (Drexel *et al.*); ●, △, ×(Kamitakahara and Brockhouse).

The frequency-versus-wave-vector dispersion relations along the symmetry directions $[00\zeta]$, $[0\zeta\zeta]$, and $[\zeta\zeta\zeta]$ of the noble metals copper, silver, and gold at room temperature are determined from solutions of secular equation (1) along these directions. The elastic constants and other relevant parameters of the metals used in the calculation are given in Table I. The resulting phonon dispersion curves are plotted in Figs. 1–3 together with experimental values obtained from recent neutron scattering experiments. In these figures L and T label the longitudinal and transverse polarization modes.

Several neutron scattering studies of lattice vibrations in copper[11-13,17-19] have been reported by many workers. However, except for the work of Sinha and Squires,[11] Svensson *et al.*,[12] and Nicklow *et al.*,[13] the results of these studies have been incomplete and somewhat inaccurate. For the purpose of comparison, we have chosen the measurements of Svensson *et al.*[12] and of Nicklow *et al.*,[13] which are in broad agreement with those of Sinha and Squires. The phonon dispersion relation in silver at room temperature has recently been reported by Drexel *et al.*[14] and by Kamitakahara and Brockhouse,[15] the latter measurements being more extensive. The experimental points of both these measurements are plotted in Fig. 2. For gold, no measurement of dispersion relations has yet been

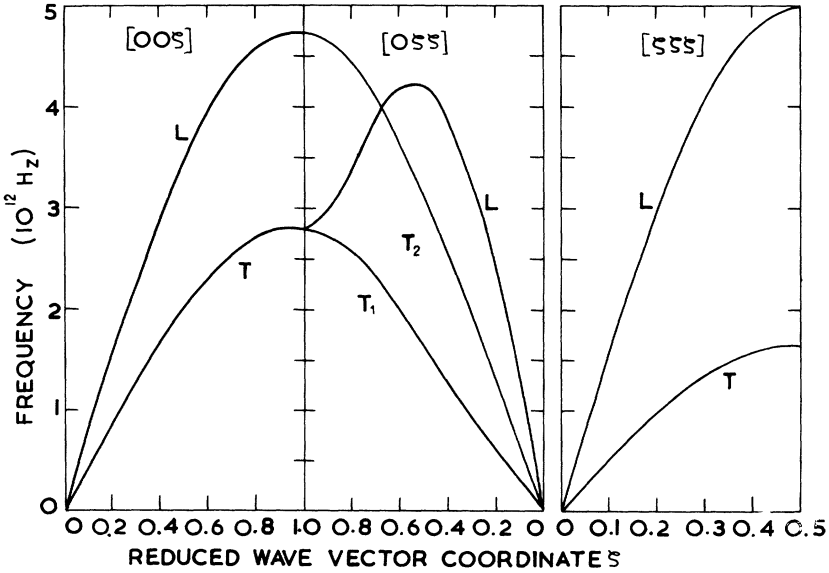

FIG. 3. Phonon dispersion curves for gold at room temperature in the three symmetry directions.

carried out.

Figures 1 and 2 show that there is reasonably satisfactory agreement between theoretical and experimental data, except for the longitudinal branches in the $[00\zeta]$ and $[\zeta\zeta\zeta]$ directions near the zone boundary. The deviations are attributable to the assumption of short-range interionic interaction in the secular equation.

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Energy Bands for KCl[†]

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Two *ab initio* calculations for KCl are reported. The first is a self-consistent Hartree-Fock calculation (accurate to first order in interatomic overlap) and the second includes correlation effects due to electron-electron interaction. The results are in excellent agreement with previous *ab initio* calculations and with experiment.

In the last two years a great deal of effort has been made by the authors, individually[1,2] and jointly,[3] in calculating the energy bands of insulating crystals from a first-principles point of view. These calculations have proved that (a) A Hartree-Fock calculation gives results which do not compare well with experiments; (b) correlation effects are very important and, after they are properly included, the agreement with experiment is very good. In this short paper we show that this is also true in the case of KCl.

Since the various techniques used in the present calculations are extensively described elsewhere[1-3] we refer the reader to those papers for details.

We proceed as follows: (a) We first perform a Hartree-Fock calculation using local orbitals[4] for the K^+ and Cl^- ion accurate to first order in interatomic overlap[5]; (b) we then include electronic correlation effects using the same procedure as in our previous works.[1,3] The method used for calculations is the mixed-basis (MB) method.[6] All the calculations were performed on the IBM 360-75 computer at the University of Illinois. The local orbital core states included in the MB method were the $1s$, $2s$, $2p$ states for both the Cl^- and K^+ states. The dielectric function $\epsilon(q)$ needed in treating correlation effects is that given in Ref. 7. The results at Γ, X, L, and Δ[8] are shown in Table I. From the Hartree-Fock results we obtain a band gap $(\Gamma_{15} \rightarrow \Gamma_1)$ of 11.76 eV; the electronic affinity is -1.69 eV; the photoemission threshold is 10.07 eV; the $3p(Cl^-)$ valence bandwidth is 3.63 eV and the $3s$ (Cl^-) band is 0.50 eV wide. When correlation effects are included, we get the values